ELSEVIER

Chemical Physics 247 (1999) 471–475

Chemical Physics

www.elsevier.nl/locate/chemphys

Author index

Aartsma, T.J., see van Oijen, A.M. 247 (1999) 53
Adachi, H., see Suzuki, C. 247 (1999) 453
Allouche, A.R., see Rousseau, S. 247 (1999) 193
Andersson, P.U., see Marković, N. 247 (1999) 413
Aubert-Frécon, M., see Rousseau, S. 247 (1999) 193

Bancewicz, M., Kurtosis of level distributions in vibrational spectra. Coupled Morse oscillators 247 (1999) 341
Basché, T., see Mais, S. 247 (1999) 41
Basché, Th., see Kulzer, F. 247 (1999) 23
Berski, S., see Lundell, J. 247 (1999) 215
Boiron, A.-M., Ph. Tamarat, B. Lounis, R. Brown and M. Orrit, Are the spectral trails of single molecules consistent with the standard two-level system model of glasses at low temperatures? 247 (1999) 119
Bondybey, V.E., see Kraus, D. 247 (1999) 431
Borin, A.C. and F.R. Ornellas, The lowest triplet and singlet electronic states of the molecule SO 247 (1999) 351
Borsenberger, P.M., see Kadashchuk, A. 247 (1999) 307
Bräuchle, C., see Mais, S. 247 (1999) 41
Brown, R., see Boiron, A.-M. 247 (1999) 119
Buckingham, A.D., see El-Sheikh, S.M. 247 (1999) 407
Burshtein, A.I., Contact and remote ion radicals formation and recombination 247 (1999) 275
Burshtein, A.I., see Krissinel, E.B. 247 (1999) 261

Cavell, R.G., see Jürgensen, A. 247 (1999) 445
Chemla, D.S., see Dahan, M. 247 (1999) 85
Chemla, D.S., see Ha, T. 247 (1999) 107
Chen, G., see Su, Z. 247 (1999) 185
Cheung, G.H., see Kowert, B.A. 247 (1999) 435
Chiu, D.T., C.F. Wilson, A. Karlsson, A. Danielsson, A. Lundqvist, A. Strömberg, F. Ryttsén, M. Davidson, S. Nordholm, O. Orwar and R.N. Zare, Manipulating the biochemical nanoenvironment around single molecules contained within vesicles 247 (1999) 133
Christ, Th., see Kulzer, F. 247 (1999) 23

Dahan, M., A.A. Deniz, T. Ha, D.S. Chemla, P.G. Schultz and S. Weiss, Ratiometric measurement and identification of single diffusing molecules 247 (1999) 85
Dang, N.C., see Kowert, B.A. 247 (1999) 435

PII: S0301-0104(99)00275-X

Danielsson, A., see Chiu, D.T. 247 (1999) 133
Dasari, R.R., see Kneipp, K. 247 (1999) 155
Davidenko, N.A. and A.A. Ishchenko, Spin conversion and electric field effect on photoluminescence in amorphous molecular semiconductors doped with ionic dyes 247 (1999) 237
Davidson, M., see Chiu, D.T. 247 (1999) 133
DeGrado, W.F., see Jia, Y. 247 (1999) 69
Deniz, A.A., see Dahan, M. 247 (1999) 85
Deniz, A.A., see Ha, T. 247 (1999) 107
Ding, S., see Zheng, Y. 247 (1999) 225
Donovan, K.J. and S. Spagnoli, Carrier range on conjugated polymers as molecular wires. Example: polydiacetylene, 4BCMU 247 (1999) 293
Duplâtre, G., see Subrahmanyam, V.S. 247 (1999) 333

Edman, L., Z. Földes-Papp, S. Wennmalm and R. Rigler, The fluctuating enzyme: a single molecule approach 247 (1999) 11
Edman, L., see Wennmalm, S. 247 (1999) 61
El-Sheikh, S.M., G.C. Tabisz and A.D. Buckingham, Collision-induced light scattering by isotropic molecules: the role of the quadrupole polarizability 247 (1999) 407
Enderlein, J., Single-molecule fluorescence near a metal layer 247 (1999) 1

Feld, M.S., see Kneipp, K. 247 (1999) 155
Ferreira Marques, M.F., see Subrahmanyam, V.S. 247 (1999) 333
Focsa, C. and B. Pinchemel, Dispersed laser-induced fluorescence of molecular ions. Identification of new low-lying electronic states of $TiCl^+$ and TiF^+ 247 (1999) 395
Földes-Papp, Z., see Edman, L. 247 (1999) 11
Francisco, J.S., see Guha, S. 247 (1999) 387
Funatsu, T., see Ishii, Y. 247 (1999) 163

Gu, Y., see Wang, B. 247 (1999) 201
Guest, M.F., see Palmer, M.H. 247 (1999) 349
Guha, S. and J.S. Francisco, A theoretical study of the isomerization pathways for $HBrO_2$ isomers 247 (1999) 387

Ha, T., A.Y. Ting, J. Liang, A.A. Deniz, D.S. Chemla, P.G. Schultz and S. Weiss, Temporal fluctuations of fluorescence resonance energy transfer between two dyes conjugated to a single protein 247 (1999) 107
Ha, T., see Dahan, M. 247 (1999) 85
Hochstrasser, R.M., see Jia, Y. 247 (1999) 69
Hou, H., see Wang, B. 247 (1999) 201
Hughes, A.M., see Kowert, B.A. 247 (1999) 435

Igoshin, O.A., see Krissinel, E.B. 247 (1999) 261
Ishchenko, A.A., see Davidenko, N.A. 247 (1999) 237
Ishii, Y., T. Yoshida, T. Funatsu, T. Wazawa and T. Yanagida, Fluorescence resonance energy transfer between single fluorophores attached to a coiled-coil protein in aqueous solution 247 (1999) 163
Itzkan, I., see Kneipp, K. 247 (1999) 155
Ivanov, A.I. and V.V. Potovoi, Theory of non-thermal electron transfer 247 (1999) 245

Jäckel, J.-G. and H. Jones, ZEKE spectroscopy of aniline–X (X = Ar, Kr, N_2 and CO) van der Waals complex cations 247 (1999) 321
Jasny, J., see Sepioł, J. 247 (1999) 35
Jastrzebski, W., see Rousseau, S. 247 (1999) 193
Jia, Y., D.S. Talaga, W.L. Lau, H.S.M. Lu, W.F. DeGrado and R.M. Hochstrasser, Folding dynamics of single GCN4 peptides by fluorescence resonant energy transfer confocal microscopy 247 (1999) 69
Jones, H., see Jäckel, J.-G. 247 (1999) 321
Jürgensen, A., N. Kosugi and R.G. Cavell, The sulphur 2p photoabsorption spectrum of NSF_3 247 (1999) 445

Kadashchuk, A., D.S. Weiss, P.M. Borsenberger, S. Nešpùrek, N. Ostapenko and V. Zaika, The origin of thermally stimulated luminescence in neat and molecularly doped charge transport polymer systems 247 (1999) 307
Karlsson, A., see Chiu, D.T. 247 (1999) 133
Kato, T., K. Yoshizawa and T. Yamabe, Vibronic coupling and Jahn–Teller effects in negatively charged [30]annulene 247 (1999) 375
Kawai, J., see Suzuki, C. 247 (1999) 453
Ketelaars, M., see van Oijen, A.M. 247 (1999) 53
Kneipp, H., see Kneipp, K. 247 (1999) 155
Kneipp, K., H. Kneipp, I. Itzkan, R.R. Dasari and M.S. Feld, Surface-enhanced non-linear Raman scattering at the single-molecule level 247 (1999) 155
Koberling, F., see Kulzer, F. 247 (1999) 23
Köhler, J., see van Oijen, A.M. 247 (1999) 53
Kortlüke, O. and W. von Niessen, Influence of hollow site adsorption in a model for the catalytic $CO + O_2$ and CO + NO reaction 247 (1999) 299
Kosugi, N., see Jürgensen, A. 247 (1999) 445
Kowalczyk, P., see Rousseau, S. 247 (1999) 193
Kowert, B.A., A.M. Hughes, N.C. Dang, M.B. Martin, G.H. Cheung, H.D. Tran and J.P. Reed, Translational diffusion of transition metal complexes 247 (1999) 435
Kraus, D., R.J. Saykally and V.E. Bondybey, Cavity ringdown spectroscopy search for transition metal dimers 247 (1999) 431
Krissinel, E.B., O.A. Igoshin and A.I. Burshtein, Integral, unified and Markovian theories of biexcitonic photoionization 247 (1999) 261
Kulzer, F., F. Koberling, Th. Christ, A. Mews and Th. Basché, Terrylene in *p*-terphenyl: single-molecule experiments at room temperature 247 (1999) 23

Latajka, Z., see Lundell, J. 247 (1999) 215
Latychevskaia, T.Yu., see Sepioł, J. 247 (1999) 35
Lau, W.L., see Jia, Y. 247 (1999) 69
Lehnert, W., E. Leiva, W. Schmickler and J.W. Schultze, A simple method for calculating the corrugation of metal surfaces 247 (1999) 207
Leiva, E., see Lehnert, W. 247 (1999) 207
Liang, J., see Ha, T. 247 (1999) 107
Liang, W., see Su, Z. 247 (1999) 185
Lounis, B., see Boiron, A.-M. 247 (1999) 119
Lu, H. and K. Schulten, Steered molecular dynamics simulation of conformational changes of immunoglobulin domain I27 interpret atomic force microscopy observations 247 (1999) 141

Lu, H.S.M., see Jia, Y. 247 (1999) 69
Lundell, J., S. Berski and Z. Latajka, Density functional study of the $Xe_2H_3^+$ cation 247 (1999) 215
Lundqvist, A., see Chiu, D.T. 247 (1999) 133

Magnier, S., see Rousseau, S. 247 (1999) 193
Mais, S., T. Basché, G. Müller, K. Müllen and C. Bräuchle, Probing the spectral dynamics of single terrylenediimide molecules in low-temperature solids 247 (1999) 41
Marković, N., P.U. Andersson, M.B. Någård and J.B.C. Pettersson, Scattering of water from graphite: simulations and experiments 247 (1999) 413
Martin, M.B., see Kowert, B.A. 247 (1999) 435
Mews, A., see Kulzer, F. 247 (1999) 23
Moc, J., Theoretical study of the CH_2Br, $CHBr_2$ and CBr_3 radicals 247 (1999) 365
Mukoyama, T., see Suzuki, C. 247 (1999) 453
Müllen, K., see Mais, S. 247 (1999) 41
Müller, G., see Mais, S. 247 (1999) 41

Någård, M.B., see Marković, N. 247 (1999) 413
Nešpùrek, S., see Kadashchuk, A. 247 (1999) 307
Nordholm, S., see Chiu, D.T. 247 (1999) 133

Onuchic, J.N., J. Wang and P.G. Wolynes, Analyzing single molecule trajectories on complex energy landscapes using replica correlation functions 247 (1999) 175
Ornellas, F.R., see Borin, A.C. 247 (1999) 351
Orrit, M., see Boiron, A.-M. 247 (1999) 119
Orwar, O., see Chiu, D.T. 247 (1999) 133
Ostapenko, N., see Kadashchuk, A. 247 (1999) 307

Palmer, M.H., I.C. Walker and M.F. Guest, Erratum to "The electronic states of thiophene studied by optical (VUV) absorption, near-threshold electron energy-loss (EEL) spectroscopy and ab initio multi-reference configuration interaction calculations". [Chemical Physics 241 (1999) 275–296] 247 (1999) 349
Pettersson, J.B.C., see Marković, N. 247 (1999) 413
Pinchemel, B., see Focsa, C. 247 (1999) 395
Potovoi, V.V., see Ivanov, A.I. 247 (1999) 245

Reed, J.P., see Kowert, B.A. 247 (1999) 435
Renn, A., see Sepioł, J. 247 (1999) 35
Rigler, R., see Edman, L. 247 (1999) 11
Rigler, R., see Wennmalm, S. 247 (1999) 61
Rousseau, S., A.R. Allouche, M. Aubert-Frécon, S. Magnier, P. Kowalczyk and W. Jastrzebski, Theoretical study of the electronic structure of KLi and comparison with experiments 247 (1999) 193
Ryttsén, F., see Chiu, D.T. 247 (1999) 133

Saykally, R.J., see Kraus, D. 247 (1999) 431
Schmickler, W., see Lehnert, W. 247 (1999) 207
Schmidt, J., see van Oijen, A.M. 247 (1999) 53
Schulten, K., see Lu, H. 247 (1999) 141
Schultz, P.G., see Dahan, M. 247 (1999) 85

Schultz, P.G., see Ha, T. 247 (1999) 107
Schultze, J.W., see Lehnert, W. 247 (1999) 207
Sepioł, J., A. Starukhin, T.Yu. Latychevskaia, J. Jasny, A. Renn and U.P. Wild, Imaging and spectroscopy of terrylene molecules isolated in vapor-deposited *n*-alkane matrices 247 (1999) 35
Spagnoli, S., see Donovan, K.J. 247 (1999) 293
Starukhin, A., see Sepioł, J. 247 (1999) 35
Strömberg, A., see Chiu, D.T. 247 (1999) 133
Su, Z., W. Liang and G. Chen, Ground-state reduced density matrices, effective Hamiltonians, and optical properties of Schiff bases of retinal 247 (1999) 185
Subrahmanyam, V.S., M.F. Ferreira Marques and G. Duplâtre, Effect of water-soluble electron scavengers on positronium formation in AOT/water/isooctane microemulsions 247 (1999) 333
Suzuki, C., J. Kawai, H. Adachi and T. Mukoyama, Electronic structures of 3d transition metal (Ti–Cu) oxides probed by a core hole 247 (1999) 453

Tabisz, G.C., see El-Sheikh, S.M. 247 (1999) 407
Talaga, D.S., see Jia, Y. 247 (1999) 69
Tamarat, Ph., see Boiron, A.-M. 247 (1999) 119
Ting, A.Y., see Ha, T. 247 (1999) 107
Tran, H.D., see Kowert, B.A. 247 (1999) 435

Van Oijen, A.M., M. Ketelaars, J. Köhler, T.J. Aartsma and J. Schmidt, Spectroscopy of individual LH2 complexes of *Rhodopseudomonas acidophila*: localized excitations in the B800 band 247 (1999) 53
Von Niessen, W., see Kortlüke, O. 247 (1999) 299

Walker, I.C., see Palmer, M.H. 247 (1999) 349
Wang, B., H. Hou and Y. Gu, Theoretical investigation of the reactions of $O(^3P)$ with CH_3F and CH_2F_2 247 (1999) 201
Wang, J., see Onuchic, J.N. 247 (1999) 175
Wazawa, T., see Ishii, Y. 247 (1999) 163
Weiss, D.S., see Kadashchuk, A. 247 (1999) 307
Weiss, S., see Dahan, M. 247 (1999) 85
Weiss, S., see Ha, T. 247 (1999) 107
Wennmalm, S., L. Edman and R. Rigler, Non-ergodic behaviour in conformational transitions of single DNA molecules 247 (1999) 61
Wennmalm, S., see Edman, L. 247 (1999) 11
Wild, U.P., see Sepioł, J. 247 (1999) 35
Wilson, C.F., see Chiu, D.T. 247 (1999) 133
Wolynes, P.G., see Onuchic, J.N. 247 (1999) 175

Yamabe, T., see Kato, T. 247 (1999) 375
Yanagida, T., see Ishii, Y. 247 (1999) 163
Yoshida, T., see Ishii, Y. 247 (1999) 163
Yoshizawa, K., see Kato, T. 247 (1999) 375

Zaika, V., see Kadashchuk, A. 247 (1999) 307
Zare, R.N., see Chiu, D.T. 247 (1999) 133
Zheng, Y. and S. Ding, Algebraic method for determining the potential energy surface for nonlinear triatomic molecules 247 (1999) 225

ELSEVIER

Chemical Physics 247 (1999) 477–488

Chemical Physics

www.elsevier.nl/locate/chemphys

Subject index

Methods and constructs

Theoretical

Computational methods for electronic structure

Manipulating the biochemical nanoenvironment around single molecules contained within vesicles, D.T. Chiu, C.F. Wilson, A. Karlsson, A. Danielsson, A. Lundqvist, A. Strömberg, F. Ryttsén, M. Davidson, S. Nordholm, O. Orwar and R.N. Zare 247 (1999) 133

Ground-state reduced density matrices, effective Hamiltonians, and optical properties of Schiff bases of retinal, Z. Su, W. Liang and G. Chen 247 (1999) 185

Theoretical study of the electronic structure of KLi and comparison with experiments, S. Rousseau, A.R. Allouche, M. Aubert-Frécon, S. Magnier, P. Kowalczyk and W. Jastrzebski 247 (1999) 193

Theoretical study of the CH_2Br, $CHBr_2$ and CBr_3 radicals, J. Moc 247 (1999) 365

Electronic structures of 3d transition metal (Ti–Cu) oxides probed by a core hole, C. Suzuki, J. Kawai, H. Adachi and T. Mukoyama 247 (1999) 453

-CI and valence bond approach

The lowest triplet and singlet electronic states of the molecule SO, A.C. Borin and F.R. Ornellas 247 (1999) 351

-perturbative and many body approaches

Theoretical investigation of the reactions of $O(^3P)$ with CH_3F and CH_2F_2, B. Wang, H. Hou and Y. Gu 247 (1999) 201

-density functional theory

A simple method for calculating the corrugation of metal surfaces, W. Lehnert, E. Leiva, W. Schmickler and J.W. Schultze 247 (1999) 207

Density functional study of the $Xe_2H_3^+$ cation, J. Lundell, S. Berski and Z. Latajka 247 (1999) 215

Theoretical study of the CH_2Br, $CHBr_2$ and CBr_3 radicals, J. Moc 247 (1999) 365

Vibronic coupling and Jahn–Teller effects in negatively charged [30]annulene, T. Kato, K. Yoshizawa and T. Yamabe 247 (1999) 375

A theoretical study of the isomerization pathways for $HBrO_2$ isomers, S. Guha and J.S. Francisco 247 (1999) 387

PII: S0301-0104(99)00276-1

Semiempirical methods
Dispersed laser-induced fluorescence of molecular ions. Identification of new low-lying electronic states of $TiCl^+$ and TiF^+, C. Focsa and B. Pinchemel 247 (1999) 395

Algebraic approaches
Algebraic method for determining the potential energy surface for nonlinear triatomic molecules, Y. Zheng and S. Ding 247 (1999) 225

Wavefunctions for highly excited and unbound states
The lowest triplet and singlet electronic states of the molecule SO, A.C. Borin and F.R. Ornellas 247 (1999) 351

Spin states and magnetic interactions
Spin conversion and electric field effect on photoluminescence in amorphous molecular semiconductors doped with ionic dyes, N.A. Davidenko and A.A. Ishchenko 247 (1999) 237

Molecular response to external fields (incl. optical susceptibilities, dichroism, hyperpolarizabilities)
Collision-induced light scattering by isotropic molecules: the role of the quadrupole polarizability, S.M. El-Sheikh, G.C. Tabisz and A.D. Buckingham 247 (1999) 407

Radiative (incl. relativistic) effects on molecules and molecular processes
Single-molecule fluorescence near a metal layer, J. Enderlein 247 (1999) 1
The fluctuating enzyme: a single molecule approach, L. Edman, Z. Földes-Papp, S. Wennmalm and R. Rigler 247 (1999) 11

Scattering of waves and particles
Scattering of water from graphite: simulations and experiments, N. Marković, P.U. Andersson, M.B. Någård and J.B.C. Pettersson 247 (1999) 413

Reactive molecular dynamics including dissipative processes
Theory of non-thermal electron transfer, A.I. Ivanov and V.V. Potovoi 247 (1999) 245

Molecular dynamics of many particle systems and condensed phases
Probing the spectral dynamics of single terrylenediimide molecules in low-temperature solids, S. Mais, T. Basché, G. Müller, K. Müllen and C. Bräuchle 247 (1999) 41
Are the spectral trails of single molecules consistent with the standard two-level system model of glasses at low temperatures?, A.-M. Boiron, Ph. Tamarat, B. Lounis, R. Brown and M. Orrit 247 (1999) 119
Steered molecular dynamics simulation of conformational changes of immunoglobulin domain I27 interpret atomic force microscopy observations, H. Lu and K. Schulten 247 (1999) 141

Quasiparticle dynamics (incl. excitons, polarons)
Integral, unified and Markovian theories of biexcitonic photoionization, E.B. Krissinel, O.A. Igoshin and A.I. Burshtein 247 (1999) 261
Contact and remote ion radicals formation and recombination, A.I. Burshtein 247 (1999) 275
Carrier range on conjugated polymers as molecular wires. Example: polydiacetylene, 4BCMU, K.J. Donovan and S. Spagnoli 247 (1999) 293

Statistical computational methods (incl. Monte Carlo)
Analyzing single molecule trajectories on complex energy landscapes using replica correlation functions, J.N. Onuchic, J. Wang and P.G. Wolynes 247 (1999) 175
Influence of hollow site adsorption in a model for the catalytic $CO + O_2$ and $CO + NO$ reaction, O. Kortlüke and W. von Niessen 247 (1999) 299

Dynamics of structures, lattices and macromolecular conformations
Folding dynamics of single GCN4 peptides by fluorescence resonant energy transfer confocal microscopy, Y. Jia, D.S. Talaga, W.L. Lau, H.S.M. Lu, W.F. DeGrado and R.M. Hochstrasser 247 (1999) 69
Analyzing single molecule trajectories on complex energy landscapes using replica correlation functions, J.N. Onuchic, J. Wang and P.G. Wolynes 247 (1999) 175

Fluctuations and random processes
Ratiometric measurement and identification of single diffusing molecules, M. Dahan, A.A. Deniz, T. Ha, D.S. Chemla, P.G. Schultz and S. Weiss 247 (1999) 85

Non-equilibrium statistical mechanics
Steered molecular dynamics simulation of conformational changes of immunoglobulin domain I27 interpret atomic force microscopy observations, H. Lu and K. Schulten 247 (1999) 141
Analyzing single molecule trajectories on complex energy landscapes using replica correlation functions, J.N. Onuchic, J. Wang and P.G. Wolynes 247 (1999) 175
Integral, unified and Markovian theories of biexcitonic photoionization, E.B. Krissinel, O.A. Igoshin and A.I. Burshtein 247 (1999) 261
Contact and remote ion radicals formation and recombination, A.I. Burshtein 247 (1999) 275

Extremum methods for ensembles (energy, entropy, free energy)
Analyzing single molecule trajectories on complex energy landscapes using replica correlation functions, J.N. Onuchic, J. Wang and P.G. Wolynes 247 (1999) 175

Experiment

Molecular spectroscopy
Terrylene in *p*-terphenyl: single-molecule experiments at room temperature, F. Kulzer, F. Koberling, Th. Christ, A. Mews and Th. Basché 247 (1999) 23
Imaging and spectroscopy of terrylene molecules isolated in vapor-deposited *n*-alkane matrices, J. Sepioł, A. Starukhin, T.Yu. Latychevskaia, J. Jasny, A. Renn and U.P. Wild 247 (1999) 35
Fluorescence resonance energy transfer between single fluorophores attached to a coiled-coil protein in aqueous solution, Y. Ishii, T. Yoshida, T. Funatsu, T. Wazawa and T. Yanagida 247 (1999) 163
The origin of thermally stimulated luminescence in neat and molecularly doped charge transport polymer systems, A. Kadashchuk, D.S. Weiss, P.M. Borsenberger, S. Nešpùrek, N. Ostapenko and V. Zaika 247 (1999) 307
Dispersed laser-induced fluorescence of molecular ions. Identification of new low-lying electronic states of $TiCl^+$ and TiF^+, C. Focsa and B. Pinchemel 247 (1999) 395
Cavity ringdown spectroscopy search for transition metal dimers, D. Kraus, R.J. Saykally and V.E. Bondybey 247 (1999) 431

-infrared
Density functional study of the $Xe_2H_3^+$ cation, J. Lundell, S. Berski and Z. Latajka 247 (1999) 215

-Raman
Surface-enhanced non-linear Raman scattering at the single-molecule level, K. Kneipp, H. Kneipp, I. Itzkan, R.R. Dasari and M.S. Feld 247 (1999) 155
Collision-induced light scattering by isotropic molecules: the role of the quadrupole polarizability, S.M. El-Sheikh, G.C. Tabisz and A.D. Buckingham 247 (1999) 407

-UV
The lowest triplet and singlet electronic states of the molecule SO, A.C. Borin and F.R. Ornellas 247 (1999) 351

-visible
Single-molecule fluorescence near a metal layer, J. Enderlein 247 (1999) 1
Terrylene in *p*-terphenyl: single-molecule experiments at room temperature, F. Kulzer, F. Koberling, Th. Christ, A. Mews and Th. Basché 247 (1999) 23
Probing the spectral dynamics of single terrylenediimide molecules in low-temperature solids, S. Mais, T. Basché, G. Müller, K. Müllen and C. Bräuchle 247 (1999) 41
Folding dynamics of single GCN4 peptides by fluorescence resonant energy transfer confocal microscopy, Y. Jia, D.S. Talaga, W.L. Lau, H.S.M. Lu, W.F. DeGrado and R.M. Hochstrasser 247 (1999) 69
Temporal fluctuations of fluorescence resonance energy transfer between two dyes conjugated to a single protein, T. Ha, A.Y. Ting, J. Liang, A.A. Deniz, D.S. Chemla, P.G. Schultz and S. Weiss 247 (1999) 107

Photon counting and phase fluorimetry
Temporal fluctuations of fluorescence resonance energy transfer between two dyes conjugated to a single protein, T. Ha, A.Y. Ting, J. Liang, A.A. Deniz, D.S. Chemla, P.G. Schultz and S. Weiss 247 (1999) 107

Multiphoton ionization
ZEKE spectroscopy of aniline–X (X = Ar, Kr, N_2 and CO) van der Waals complex cations, J.-G. Jäckel and H. Jones 247 (1999) 321

X-ray spectroscopy
The sulphur 2p photoabsorption spectrum of NSF_3, A. Jürgensen, N. Kosugi and R.G. Cavell 247 (1999) 445

Electron impact spectroscopy
Spin conversion and electric field effect on photoluminescence in amorphous molecular semiconductors doped with ionic dyes, N.A. Davidenko and A.A. Ishchenko 247 (1999) 237

Laser induced fluorescence
The fluctuating enzyme: a single molecule approach, L. Edman, Z. Földes-Papp, S. Wennmalm and R. Rigler 247 (1999) 11
Imaging and spectroscopy of terrylene molecules isolated in vapor-deposited *n*-alkane matrices, J. Sepioł, A. Starukhin, T.Yu. Latychevskaia, J. Jasny, A. Renn and U.P. Wild 247 (1999) 35

Spectroscopy of individual LH2 complexes of *Rhodopseudomonas acidophila*: localized excitations in the B800 band, A.M. van Oijen, M. Ketelaars, J. Köhler, T.J. Aartsma and J. Schmidt 247 (1999) 53
Non-ergodic behaviour in conformational transitions of single DNA molecules, S. Wennmalm, L. Edman and R. Rigler 247 (1999) 61
Ratiometric measurement and identification of single diffusing molecules, M. Dahan, A.A. Deniz, T. Ha, D.S. Chemla, P.G. Schultz and S. Weiss 247 (1999) 85
Are the spectral trails of single molecules consistent with the standard two-level system model of glasses at low temperatures?, A.-M. Boiron, Ph. Tamarat, B. Lounis, R. Brown and M. Orrit 247 (1999) 119
Manipulating the biochemical nanoenvironment around single molecules contained within vesicles, D.T. Chiu, C.F. Wilson, A. Karlsson, A. Danielsson, A. Lundqvist, A. Strömberg, F. Ryttsén, M. Davidson, S. Nordholm, O. Orwar and R.N. Zare 247 (1999) 133
Dispersed laser-induced fluorescence of molecular ions. Identification of new low-lying electronic states of $TiCl^+$ and TiF^+, C. Focsa and B. Pinchemel 247 (1999) 395

Ultrafast measurements
Effect of water-soluble electron scavengers on positronium formation in AOT/water/isooctane microemulsions, V.S. Subrahmanyam, M.F. Ferreira Marques and G. Duplâtre 247 (1999) 333

Atomic and molecular beam techniques
Scattering of water from graphite: simulations and experiments, N. Marković, P.U. Andersson, M.B. Någård and J.B.C. Pettersson 247 (1999) 413
Cavity ringdown spectroscopy search for transition metal dimers, D. Kraus, R.J. Saykally and V.E. Bondybey 247 (1999) 431

Mass spectroscopy
A theoretical study of the isomerization pathways for $HBrO_2$ isomers, S. Guha and J.S. Francisco 247 (1999) 387

Radiolysis
Carrier range on conjugated polymers as molecular wires. Example: polydiacetylene, 4BCMU, K.J. Donovan and S. Spagnoli 247 (1999) 293

Objects

Bulk systems

Gases
Theoretical investigation of the reactions of $O(^3P)$ with CH_3F and CH_2F_2, B. Wang, H. Hou and Y. Gu 247 (1999) 201
A theoretical study of the isomerization pathways for $HBrO_2$ isomers, S. Guha and J.S. Francisco 247 (1999) 387
Collision-induced light scattering by isotropic molecules: the role of the quadrupole polarizability, S.M. El-Sheikh, G.C. Tabisz and A.D. Buckingham 247 (1999) 407
The sulphur 2p photoabsorption spectrum of NSF_3, A. Jürgensen, N. Kosugi and R.G. Cavell 247 (1999) 445

Liquid mixtures and solutions
Integral, unified and Markovian theories of biexcitonic photoionization, E.B. Krissinel, O.A. Igoshin and A.I. Burshtein 247 (1999) 261
Effect of water-soluble electron scavengers on positronium formation in AOT/water/iso-octane microemulsions, V.S. Subrahmanyam, M.F. Ferreira Marques and G. Duplâtre 247 (1999) 333
Translational diffusion of transition metal complexes, B.A. Kowert, A.M. Hughes, N.C. Dang, M.B. Martin, G.H. Cheung, H.D. Tran and J.P. Reed 247 (1999) 435

Crystals
Terrylene in *p*-terphenyl: single-molecule experiments at room temperature, F. Kulzer, F. Koberling, Th. Christ, A. Mews and Th. Basché 247 (1999) 23
Carrier range on conjugated polymers as molecular wires. Example: polydiacetylene, 4BCMU, K.J. Donovan and S. Spagnoli 247 (1999) 293

-mixed
Terrylene in *p*-terphenyl: single-molecule experiments at room temperature, F. Kulzer, F. Koberling, Th. Christ, A. Mews and Th. Basché 247 (1999) 23
Imaging and spectroscopy of terrylene molecules isolated in vapor-deposited *n*-alkane matrices, J. Sepioł, A. Starukhin, T.Yu. Latychevskaia, J. Jasny, A. Renn and U.P. Wild 247 (1999) 35
Density functional study of the $Xe_2H_3^+$ cation, J. Lundell, S. Berski and Z. Latajka 247 (1999) 215

Complex fluids
Effect of water-soluble electron scavengers on positronium formation in AOT/water/iso-octane microemulsions, V.S. Subrahmanyam, M.F. Ferreira Marques and G. Duplâtre 247 (1999) 333

Polymers
Probing the spectral dynamics of single terrylenediimide molecules in low-temperature solids, S. Mais, T. Basché, G. Müller, K. Müllen and C. Bräuchle 247 (1999) 41
Are the spectral trails of single molecules consistent with the standard two-level system model of glasses at low temperatures?, A.-M. Boiron, Ph. Tamarat, B. Lounis, R. Brown and M. Orrit 247 (1999) 119
The origin of thermally stimulated luminescence in neat and molecularly doped charge transport polymer systems, A. Kadashchuk, D.S. Weiss, P.M. Borsenberger, S. Nešpůrek, N. Ostapenko and V. Zaika 247 (1999) 307

Semiconductors
Spin conversion and electric field effect on photoluminescence in amorphous molecular semiconductors doped with ionic dyes, N.A. Davidenko and A.A. Ishchenko 247 (1999) 237

Metals and alloys
Cavity ringdown spectroscopy search for transition metal dimers, D. Kraus, R.J. Saykally and V.E. Bondybey 247 (1999) 431

Surfaces
A simple method for calculating the corrugation of metal surfaces, W. Lehnert, E. Leiva, W. Schmickler and J.W. Schultze 247 (1999) 207
Influence of hollow site adsorption in a model for the catalytic $CO + O_2$ and $CO + NO$ reaction, O. Kortlüke and W. von Niessen 247 (1999) 299

Biological systems
The fluctuating enzyme: a single molecule approach, L. Edman, Z. Földes-Papp, S. Wennmalm and R. Rigler 247 (1999) 11
Spectroscopy of individual LH2 complexes of *Rhodopseudomonas acidophila*: localized excitations in the B800 band, A.M. van Oijen, M. Ketelaars, J. Köhler, T.J. Aartsma and J. Schmidt 247 (1999) 53
Folding dynamics of single GCN4 peptides by fluorescence resonant energy transfer confocal microscopy, Y. Jia, D.S. Talaga, W.L. Lau, H.S.M. Lu, W.F. DeGrado and R.M. Hochstrasser 247 (1999) 69
Manipulating the biochemical nanoenvironment around single molecules contained within vesicles, D.T. Chiu, C.F. Wilson, A. Karlsson, A. Danielsson, A. Lundqvist, A. Strömberg, F. Ryttsén, M. Davidson, S. Nordholm, O. Orwar and R.N. Zare 247 (1999) 133

Microscopic and mesoscopic systems

Single atoms, molecules and assemblies (incl. biological)
Single-molecule fluorescence near a metal layer, J. Enderlein 247 (1999) 1
The fluctuating enzyme: a single molecule approach, L. Edman, Z. Földes-Papp, S. Wennmalm and R. Rigler 247 (1999) 11
Terrylene in *p*-terphenyl: single-molecule experiments at room temperature, F. Kulzer, F. Koberling, Th. Christ, A. Mews and Th. Basché 247 (1999) 23
Imaging and spectroscopy of terrylene molecules isolated in vapor-deposited *n*-alkane matrices, J. Sepioł, A. Starukhin, T.Yu. Latychevskaia, J. Jasny, A. Renn and U.P. Wild 247 (1999) 35
Probing the spectral dynamics of single terrylenediimide molecules in low-temperature solids, S. Mais, T. Basché, G. Müller, K. Müllen and C. Bräuchle 247 (1999) 41
Ratiometric measurement and identification of single diffusing molecules, M. Dahan, A.A. Deniz, T. Ha, D.S. Chemla, P.G. Schultz and S. Weiss 247 (1999) 85
Temporal fluctuations of fluorescence resonance energy transfer between two dyes conjugated to a single protein, T. Ha, A.Y. Ting, J. Liang, A.A. Deniz, D.S. Chemla, P.G. Schultz and S. Weiss 247 (1999) 107
Are the spectral trails of single molecules consistent with the standard two-level system model of glasses at low temperatures?, A.-M. Boiron, Ph. Tamarat, B. Lounis, R. Brown and M. Orrit 247 (1999) 119
Manipulating the biochemical nanoenvironment around single molecules contained within vesicles, D.T. Chiu, C.F. Wilson, A. Karlsson, A. Danielsson, A. Lundqvist, A. Strömberg, F. Ryttsén, M. Davidson, S. Nordholm, O. Orwar and R.N. Zare 247 (1999) 133
Surface-enhanced non-linear Raman scattering at the single-molecule level, K. Kneipp, H. Kneipp, I. Itzkan, R.R. Dasari and M.S. Feld 247 (1999) 155
Fluorescence resonance energy transfer between single fluorophores attached to a coiled-coil protein in aqueous solution, Y. Ishii, T. Yoshida, T. Funatsu, T. Wazawa and T. Yanagida 247 (1999) 163

Molecules (neutral and ionic)
Ground-state reduced density matrices, effective Hamiltonians, and optical properties of Schiff bases of retinal, Z. Su, W. Liang and G. Chen 247 (1999) 185
Theory of non-thermal electron transfer, A.I. Ivanov and V.V. Potovoi 247 (1999) 245

The origin of thermally stimulated luminescence in neat and molecularly doped charge transport polymer systems, A. Kadashchuk, D.S. Weiss, P.M. Borsenberger, S. Nešpůrek, N. Ostapenko and V. Zaika 247 (1999) 307
Kurtosis of level distributions in vibrational spectra. Coupled Morse oscillators, M. Bancewicz 247 (1999) 341

-diatomic
Theoretical study of the electronic structure of KLi and comparison with experiments, S. Rousseau, A.R. Allouche, M. Aubert-Frécon, S. Magnier, P. Kowalczyk and W. Jastrzebski 247 (1999) 193
The lowest triplet and singlet electronic states of the molecule SO, A.C. Borin and F.R. Ornellas 247 (1999) 351
Dispersed laser-induced fluorescence of molecular ions. Identification of new low-lying electronic states of $TiCl^+$ and TiF^+, C. Focsa and B. Pinchemel 247 (1999) 395

-small polyatomics
Density functional study of the $Xe_2H_3^+$ cation, J. Lundell, S. Berski and Z. Latajka 247 (1999) 215
Algebraic method for determining the potential energy surface for nonlinear triatomic molecules, Y. Zheng and S. Ding 247 (1999) 225
Scattering of water from graphite: simulations and experiments, N. Marković, P.U. Andersson, M.B. Någård and J.B.C. Pettersson 247 (1999) 413
The sulphur 2p photoabsorption spectrum of NSF_3, A. Jürgensen, N. Kosugi and R.G. Cavell 247 (1999) 445

-aromatics
Imaging and spectroscopy of terrylene molecules isolated in vapor-deposited *n*-alkane matrices, J. Sepioł, A. Starukhin, T.Yu. Latychevskaia, J. Jasny, A. Renn and U.P. Wild 247 (1999) 35
Are the spectral trails of single molecules consistent with the standard two-level system model of glasses at low temperatures?, A.-M. Boiron, Ph. Tamarat, B. Lounis, R. Brown and M. Orrit 247 (1999) 119
Vibronic coupling and Jahn–Teller effects in negatively charged [30]annulene, T. Kato, K. Yoshizawa and T. Yamabe 247 (1999) 375

-polymeric and biological
Carrier range on conjugated polymers as molecular wires. Example: polydiacetylene, 4BCMU, K.J. Donovan and S. Spagnoli 247 (1999) 293

Molecular aggregates
Collision-induced light scattering by isotropic molecules: the role of the quadrupole polarizability, S.M. El-Sheikh, G.C. Tabisz and A.D. Buckingham 247 (1999) 407

-dimers
Cavity ringdown spectroscopy search for transition metal dimers, D. Kraus, R.J. Saykally and V.E. Bondybey 247 (1999) 431

-van der Waals molecules
ZEKE spectroscopy of aniline–X (X = Ar, Kr, N_2 and CO) van der Waals complex cations, J.-G. Jäckel and H. Jones 247 (1999) 321

-clusters
Electronic structures of 3d transition metal (Ti–Cu) oxides probed by a core hole, C. Suzuki, J. Kawai, H. Adachi and T. Mukoyama 247 (1999) 453

-complexes
A theoretical study of the isomerization pathways for $HBrO_2$ isomers, S. Guha and J.S. Francisco 247 (1999) 387

Ions and charge carriers
ZEKE spectroscopy of aniline–X (X = Ar, Kr, N_2 and CO) van der Waals complex cations, J.-G. Jäckel and H. Jones 247 (1999) 321

Biological assemblies, cells and organelles
Folding dynamics of single GCN4 peptides by fluorescence resonant energy transfer confocal microscopy, Y. Jia, D.S. Talaga, W.L. Lau, H.S.M. Lu, W.F. DeGrado and R.M. Hochstrasser 247 (1999) 69

Proteins
Temporal fluctuations of fluorescence resonance energy transfer between two dyes conjugated to a single protein, T. Ha, A.Y. Ting, J. Liang, A.A. Deniz, D.S. Chemla, P.G. Schultz and S. Weiss 247 (1999) 107
Steered molecular dynamics simulation of conformational changes of immunoglobulin domain I27 interpret atomic force microscopy observations, H. Lu and K. Schulten 247 (1999) 141
Fluorescence resonance energy transfer between single fluorophores attached to a coiled-coil protein in aqueous solution, Y. Ishii, T. Yoshida, T. Funatsu, T. Wazawa and T. Yanagida 247 (1999) 163

Nucleic acids
Non-ergodic behaviour in conformational transitions of single DNA molecules, S. Wennmalm, L. Edman and R. Rigler 247 (1999) 61

Phenomena

Molecular structure
Density functional study of the $Xe_2H_3^+$ cation, J. Lundell, S. Berski and Z. Latajka 247 (1999) 215
Algebraic method for determining the potential energy surface for nonlinear triatomic molecules, Y. Zheng and S. Ding 247 (1999) 225
Theoretical study of the CH_2Br, $CHBr_2$ and CBr_3 radicals, J. Moc 247 (1999) 365
A theoretical study of the isomerization pathways for $HBrO_2$ isomers, S. Guha and J.S. Francisco 247 (1999) 387

Vibrations and rotations of molecules
Algebraic method for determining the potential energy surface for nonlinear triatomic molecules, Y. Zheng and S. Ding 247 (1999) 225
Kurtosis of level distributions in vibrational spectra. Coupled Morse oscillators, M. Bancewicz 247 (1999) 341

Theoretical study of the CH_2Br, $CHBr_2$ and CBr_3 radicals, J. Moc 247 (1999) 365
Cavity ringdown spectroscopy search for transition metal dimers, D. Kraus, R.J. Saykally and V.E. Bondybey 247 (1999) 431

Electronic structure and states
Ground-state reduced density matrices, effective Hamiltonians, and optical properties of Schiff bases of retinal, Z. Su, W. Liang and G. Chen 247 (1999) 185
Theoretical study of the electronic structure of KLi and comparison with experiments, S. Rousseau, A.R. Allouche, M. Aubert-Frécon, S. Magnier, P. Kowalczyk and W. Jastrzebski 247 (1999) 193
A simple method for calculating the corrugation of metal surfaces, W. Lehnert, E. Leiva, W. Schmickler and J.W. Schultze 247 (1999) 207
The lowest triplet and singlet electronic states of the molecule SO, A.C. Borin and F.R. Ornellas 247 (1999) 351
Dispersed laser-induced fluorescence of molecular ions. Identification of new low-lying electronic states of $TiCl^+$ and TiF^+, C. Focsa and B. Pinchemel 247 (1999) 395
Electronic structures of 3d transition metal (Ti–Cu) oxides probed by a core hole, C. Suzuki, J. Kawai, H. Adachi and T. Mukoyama 247 (1999) 453
The sulphur 2p photoabsorption spectrum of NSF_3, A. Jürgensen, N. Kosugi and R.G. Cavell 247 (1999) 445

Molecular interactions
Translational diffusion of transition metal complexes, B.A. Kowert, A.M. Hughes, N.C. Dang, M.B. Martin, G.H. Cheung, H.D. Tran and J.P. Reed 247 (1999) 435

Spectral bandshapes and intensities
Probing the spectral dynamics of single terrylenediimide molecules in low-temperature solids, S. Mais, T. Basché, G. Müller, K. Müllen and C. Bräuchle 247 (1999) 41
Collision-induced light scattering by isotropic molecules: the role of the quadrupole polarizability, S.M. El-Sheikh, G.C. Tabisz and A.D. Buckingham 247 (1999) 407

Coupling of electronic and nuclear motion
Vibronic coupling and Jahn–Teller effects in negatively charged [30]annulene, T. Kato, K. Yoshizawa and T. Yamabe 247 (1999) 375

Energy transfer processes
Non-ergodic behaviour in conformational transitions of single DNA molecules, S. Wennmalm, L. Edman and R. Rigler 247 (1999) 61
Ratiometric measurement and identification of single diffusing molecules, M. Dahan, A.A. Deniz, T. Ha, D.S. Chemla, P.G. Schultz and S. Weiss 247 (1999) 85
Temporal fluctuations of fluorescence resonance energy transfer between two dyes conjugated to a single protein, T. Ha, A.Y. Ting, J. Liang, A.A. Deniz, D.S. Chemla, P.G. Schultz and S. Weiss 247 (1999) 107
Fluorescence resonance energy transfer between single fluorophores attached to a coiled-coil protein in aqueous solution, Y. Ishii, T. Yoshida, T. Funatsu, T. Wazawa and T. Yanagida 247 (1999) 163
Scattering of water from graphite: simulations and experiments, N. Marković, P.U. Andersson, M.B. Någård and J.B.C. Pettersson 247 (1999) 413

Molecular photophysical processes
Single-molecule fluorescence near a metal layer, J. Enderlein 247 (1999) 1
Terrylene in *p*-terphenyl: single-molecule experiments at room temperature, F. Kulzer, F. Koberling, Th. Christ, A. Mews and Th. Basché 247 (1999) 23
Spin conversion and electric field effect on photoluminescence in amorphous molecular semiconductors doped with ionic dyes, N.A. Davidenko and A.A. Ishchenko 247 (1999) 237

Photochemistry
Integral, unified and Markovian theories of biexcitonic photoionization, E.B. Krissinel, O.A. Igoshin and A.I. Burshtein 247 (1999) 261
Contact and remote ion radicals formation and recombination, A.I. Burshtein 247 (1999) 275

Intramolecular dynamics

-protein motion
The fluctuating enzyme: a single molecule approach, L. Edman, Z. Földes-Papp, S. Wennmalm and R. Rigler 247 (1999) 11
Steered molecular dynamics simulation of conformational changes of immunoglobulin domain I27 interpret atomic force microscopy observations, H. Lu and K. Schulten 247 (1999) 141

Luminescence spectra, yields and lifetimes
Single-molecule fluorescence near a metal layer, J. Enderlein 247 (1999) 1
Integral, unified and Markovian theories of biexcitonic photoionization, E.B. Krissinel, O.A. Igoshin and A.I. Burshtein 247 (1999) 261
Contact and remote ion radicals formation and recombination, A.I. Burshtein 247 (1999) 275
The origin of thermally stimulated luminescence in neat and molecularly doped charge transport polymer systems, A. Kadashchuk, D.S. Weiss, P.M. Borsenberger, S. Nešpùrek, N. Ostapenko and V. Zaika 247 (1999) 307

Nonlinear responses (incl. optical)
Surface-enhanced non-linear Raman scattering at the single-molecule level, K. Kneipp, H. Kneipp, I. Itzkan, R.R. Dasari and M.S. Feld 247 (1999) 155

Reactions (incl. dissociation)
Theoretical investigation of the reactions of $O(^3P)$ with CH_3F and CH_2F_2, B. Wang, H. Hou and Y. Gu 247 (1999) 201

Tunneling
Theoretical investigation of the reactions of $O(^3P)$ with CH_3F and CH_2F_2, B. Wang, H. Hou and Y. Gu 247 (1999) 201

Electron transfer
Theory of non-thermal electron transfer, A.I. Ivanov and V.V. Potovoi 247 (1999) 245
Carrier range on conjugated polymers as molecular wires. Example: polydiacetylene, 4BCMU, K.J. Donovan and S. Spagnoli 247 (1999) 293

Positron annihilation
Effect of water-soluble electron scavengers on positronium formation in AOT/water/iso-octane microemulsions, V.S. Subrahmanyam, M.F. Ferreira Marques and G. Duplâtre 247 (1999) 333

Molecular motion (incl. diffusive)
Translational diffusion of transition metal complexes, B.A. Kowert, A.M. Hughes, N.C. Dang, M.B. Martin, G.H. Cheung, H.D. Tran and J.P. Reed 247 (1999) 435

Isotopic effects
Vibronic coupling and Jahn–Teller effects in negatively charged [30]annulene, T. Kato, K. Yoshizawa and T. Yamabe 247 (1999) 375

Fluctuations and noise
Folding dynamics of single GCN4 peptides by fluorescence resonant energy transfer confocal microscopy, Y. Jia, D.S. Talaga, W.L. Lau, H.S.M. Lu, W.F. DeGrado and R.M. Hochstrasser 247 (1999) 69
Ratiometric measurement and identification of single diffusing molecules, M. Dahan, A.A. Deniz, T. Ha, D.S. Chemla, P.G. Schultz and S. Weiss 247 (1999) 85

Surface chemical physics

-surface scattering
Scattering of water from graphite: simulations and experiments, N. Marković, P.U. Andersson, M.B. Någård and J.B.C. Pettersson 247 (1999) 413

-adsorbate structure
Influence of hollow site adsorption in a model for the catalytic $CO + O_2$ and $CO + NO$ reaction, O. Kortlüke and W. von Niessen 247 (1999) 299

-surface reactions
Influence of hollow site adsorption in a model for the catalytic $CO + O_2$ and $CO + NO$ reaction, O. Kortlüke and W. von Niessen 247 (1999) 299

Critical behavior and phase transitions
Influence of hollow site adsorption in a model for the catalytic $CO + O_2$ and $CO + NO$ reaction, O. Kortlüke and W. von Niessen 247 (1999) 299

Biomolecular structure–function relationships
Steered molecular dynamics simulation of conformational changes of immunoglobulin domain I27 interpret atomic force microscopy observations, H. Lu and K. Schulten 247 (1999) 141